Dodecane 112-40-3 | DTXSID0026913

Model Performance

| M. J. I | D. L. |
|---------|-------|
| Model | Data |
| 110001 | Bata |

Weighted KNN model

| 5-fold CV (| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-------------|-----------------|------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 | |

Model Results

Predicted value: 10.6 days

Global applicability domain: Inside

Local applicability domain index: 8.88e-01

Confidence level: 8.89e-01

Nearest Neighbors from the Training Set

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Dodecane Measured: 201 Predicted: 10.6 Image not found

Tridecane Measured: 305 Predicted: 13.5 Image not found

Undecane Measured: 88.3 Predicted: 8.56

Image not found

Tetradecane
Measured: 1370
Predicted: 18.3

Image not found

Decane
Measured: 157
Predicted: 8.71